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UNEP/ SETAC partnership to advance the life cycle economy

Development in methodologies for modelling of human and ecotoxic impacts in LCA

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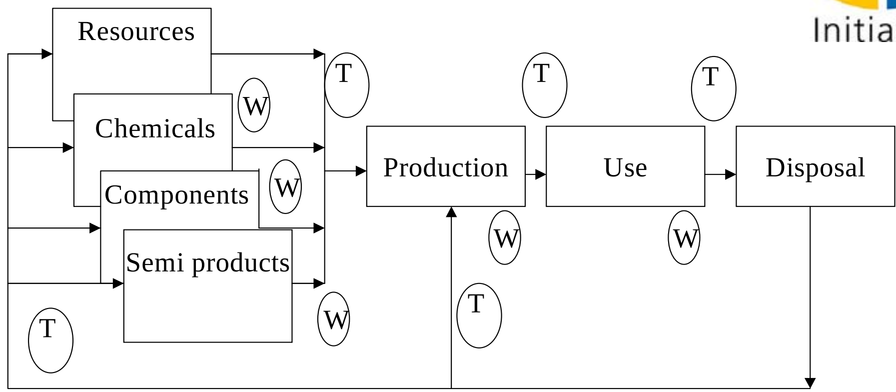
Inventory of emissions

		Emission	Emission
	CAS.no.	to air	to w ater
Substance		g	g
2-hydroxy-ethanacrylate	816-61-0	0,0348	
4,4-methylenebis cyclohexylamine	1761-71-2	5,9E-02	
Ammonia	7664-81-7	3,7E-05	4,2E-05
Arsenic (As)	7440-38-2	2,0E-06	
Benzene	71-43-2 (cur	5,0E-02	
Lead (Pb)	7439-92-1	8,5E-06	
Butoxyethanol	111-76-2	6,6E-01	
Carbondioxide	124-38-9	2,6E+02	
Carbonmonoxide (CO)	630-08-0	1,9E-01	
Cadmium (Cd)	7440-46-9	2,2E-07	
Chlorine (Cl2)	7782-50-5	4,6E-04	
Chromium (Cr VI)	7440-47-3	5,3E-06	
Dicyclohexane methane	86-73-6	5,1E-02	
Nitrous oxide(N2O)	10024-97-2	1,7E-02	
2,4-Dinitrotoluene	121-14-2	9,5E-02	
HMDI	5124-30-1	7,5E-02	
Hydro carbons (electricity, stationary combustic	-	1,7E+00	
Hydrogen ions (H+)	-		1,0E-03
i-butanol	78-83-1	3,5E-02	
i-propanol	67-63-0	9,2E-01	
copper (Cu)	7740-50-8	1,8E-05	
Mercury(Hg)	7439-97-6	2,7E-06	
Methane	74-82-8	5,0E-03	
Methyl i-butyl ketone	108-10-1	5,7E-02	
Monoethyl amine	75-04-7		7,9E-06
Nickel (Ni)	7440-02-0	1,1E-05	
Nitrogen oxide (NOx)	10102-44-0	1,1E+00	
NMVOC, diesel engine (exhaust)	-	3,9E-02	
NMVOC, pow er plants (stationary combustion)	-	3,9E-03	
Ozone (O3)	10028-15-6	1,8E-03	
PAH	ikke specifik	2,4E-08	
Phenol	108-95-2		1,3E-05
Phosgene	75-44-5	1,4E-01	
Polyeter polyol	ikke specifik	1,6E-01	
1,2-propylenoxide	75-56-9	8,2E-02	
Nitric acid	7782-77-6 (c	8,5E-02	
Hydrochloric acid	7647-01-0 (c	1,9E-02	
Selenium (Se)	7782-49-2	2,6E-05	
Sulphur dioxide(SO2)	7446-09-5	1,3E+00	
Toluene	108-88-3	4,8E-02	
Toluene-2,4-diamine	95-80-7	7,9E-02	
Toluene diisocyanat (TDI)	26471-62-5	1,6E-01	
Total-N	-		2,6E-05
Triethylamine	121-44-8	1,6E-01	
Unspecified aldehydes	-	7,5E-04	
Uspecified organic compounds	-	1,5E-03	
Vanadium	7440-62-2	1,8E-04	
VOC, diesel engine (exhaust)	-	6,4E-05	
VOC, stationary combustion (coal fired)	-	4,0E-05	
VOC, stationary combustion (natural gas fired)	-	2,2E-03	
VOC, stationary combustion (oil fired)	-	1,4E-04	
Xylene	1330-20-7	1,4E-01	
Zinc (Zn)	7440-66-6	8,9E-05	

The product life cycle



Characterised impact profile of product

Global warming	174.000	kg CO_2-eq
Ozone depletion	0	kg CFC11-eq
Acidification	868	kg SO_2-eq
Photochemical ozone formation	200	kg C_2H_4-eq
Nutrient enrichment	3.576	kg NO_3^--eq
Human toxicity	$3,40 \cdot 10^{11}$	m^3 air
Ecotoxicity	$2,16 \cdot 10^{7}$	m^3 water
Land use	170	ha·yr
Volume waste	9.450	kg
Hazardous waste	248	kg

Background

- Characterisation factors (CFs) express potential impact on human health or ecosystems
- For comparison of chemicals (relative scale)
- Different characterisation methods give very different results
- CFs missing for many of the substances encountered in inventories for products
- → unsatisfactory treatment of chemicals in LCA
- Chemicals often not included in Life Cycle Impact Assessments (LCIAs)
- Results often inconclusive
- … Environmental LCA in practice often Energy LCA

About the *Life Cycle Initiative*

Joint initiative between United Nations Environment Programme (UNEP) and Society of Environmental Toxicology and Chemistry (SETAC):

Enhancement of the availability of sound LCA data and methods and guidance about their use.

For toxic impacts:

Recommended characterisation models and factors for human toxicity and ecotoxicity

- applicable on a world-wide basis
- for a large number of substances

Goal

- Identification of good modelling practice
- Harmonisation of existing models
- Recommendation of characterisation model
- Recommendation of characterisation factors
- Provision of characterisation factors for many substances
- Guidance on use of characterisation factors

LCIA and ERA of chemicals

Similarities

- Multimedia, multi compartment fate and exposure models
- Same type of physico-chemical and biological substance data (Kow, H, DT50, EC50, …)

Differences:

	ERA	LCIA
Scope of impacts	Chemical exposure of humans and ecosystems	All known environmental impacts
Scope of substances	Focused on one or a few substances	Focused on life cycle inventory (hundreds of substances)
Issue addressed	Is there a risk of critical exposure?	Largest potential impact - A or B? How much larger?
Modelling assumptions and parameter choices	Conservative assumptions ("realistic worst case)	Best estimate (avoid bias in comparison with other impacts)
Spatial differentiation	Often site-*dependent*	Normally site-*generic*

Process

- Consensus created through joint efforts on
  - Identification of state of the art
  - Identification of good modelling practice
  - … Monthly teleconferences keep the process going
- Review workshops with external experts
- Need for model comparison identified
- Need for consensus model identified
- Sponsorship obtained
  - ICMM
  - ACC
  - UNEP
- … seed money which supported a huge voluntary effort from the participants

Model comparison

Existing models compared on their results and main sources of differences in their output identified

- CalTOX **(McKone et al., USA)**
- IMPACT 2002 **(Pennington et al., Switzerland)**
- USES-LCA **(Huijbregts et al., Netherlands)**
- BETR **(MacLeod et al., Canada)**
- EDIP **(Hauschild et al., Denmark)**
- WATSON **(Bachmann et al., Germany)**
- EcoSense **(Droste-Franke et al., Germany)**

3 expert review workshops and 3 model comparison workshops

Using a test set with broad organic chemical representation

Main sources of difference identified, unintentional sources eliminated

A UNEP/SETAC toxicity scientific consensus model created – **USEtox™**

The principles behind USEtox™

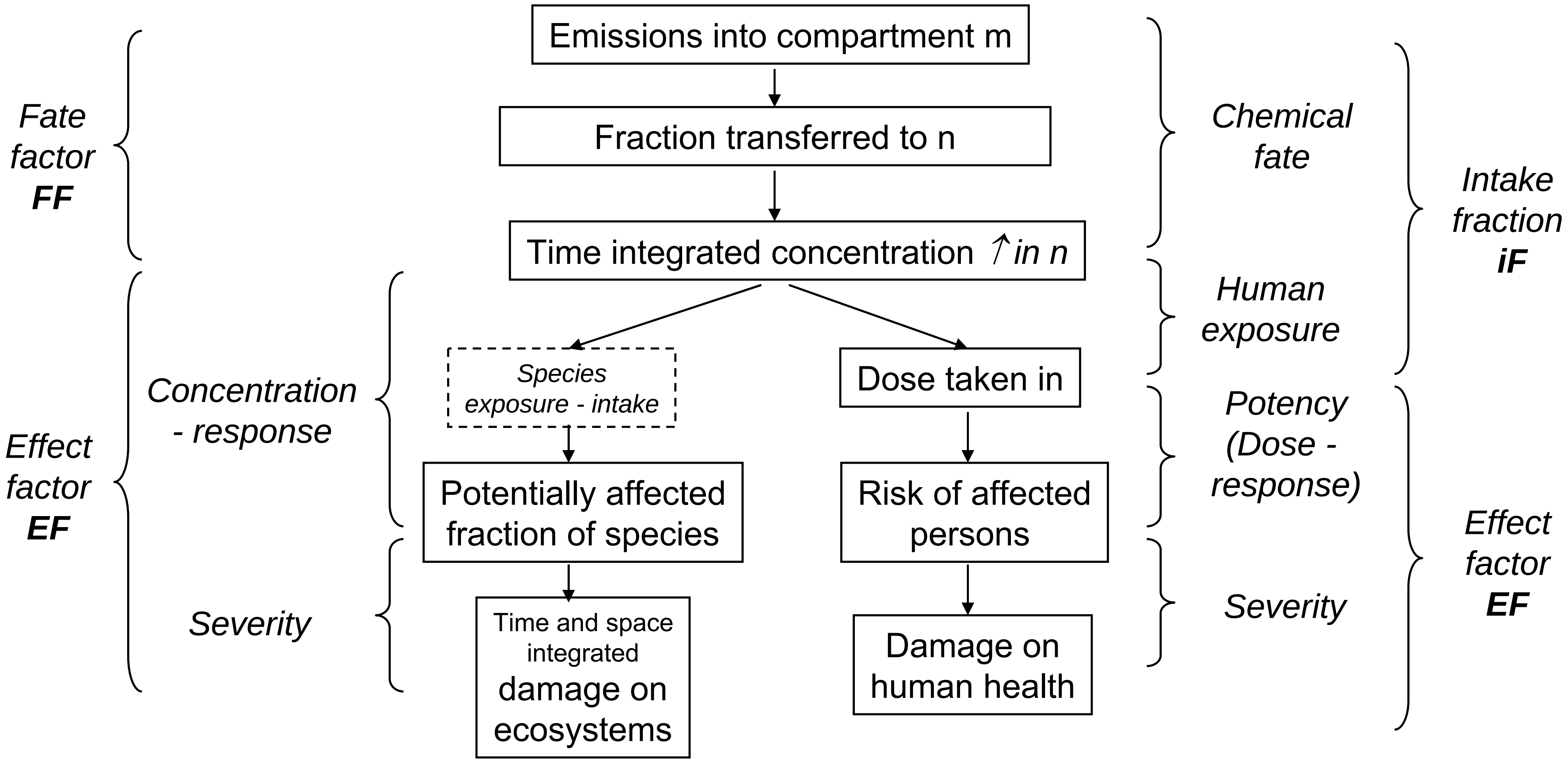
Parsimonious **– as simple as possible but as complex as needed – containing only the most influential model components;**

Mimetic **– not differing more from the original models than these differ among themselves;**

Evaluated **– providing a repository of knowledge through evaluation against existing models;**

Transparent **– being well documented, including the reasoning for model choices.**

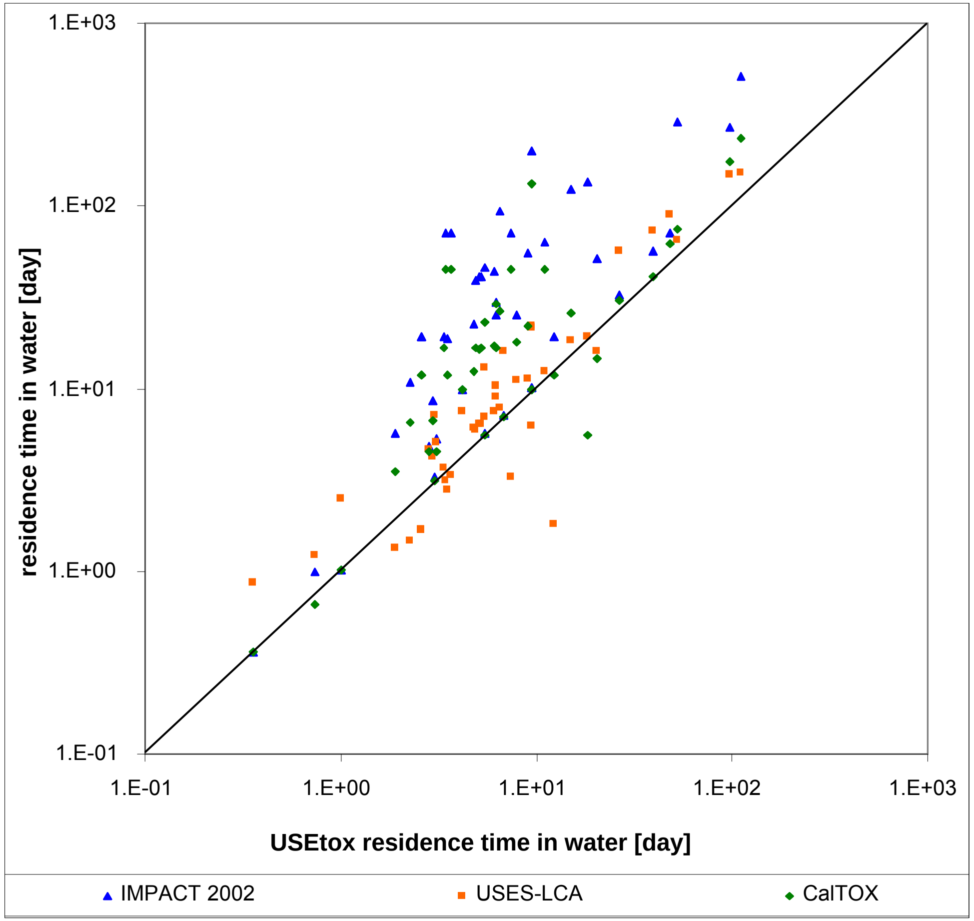
Framework

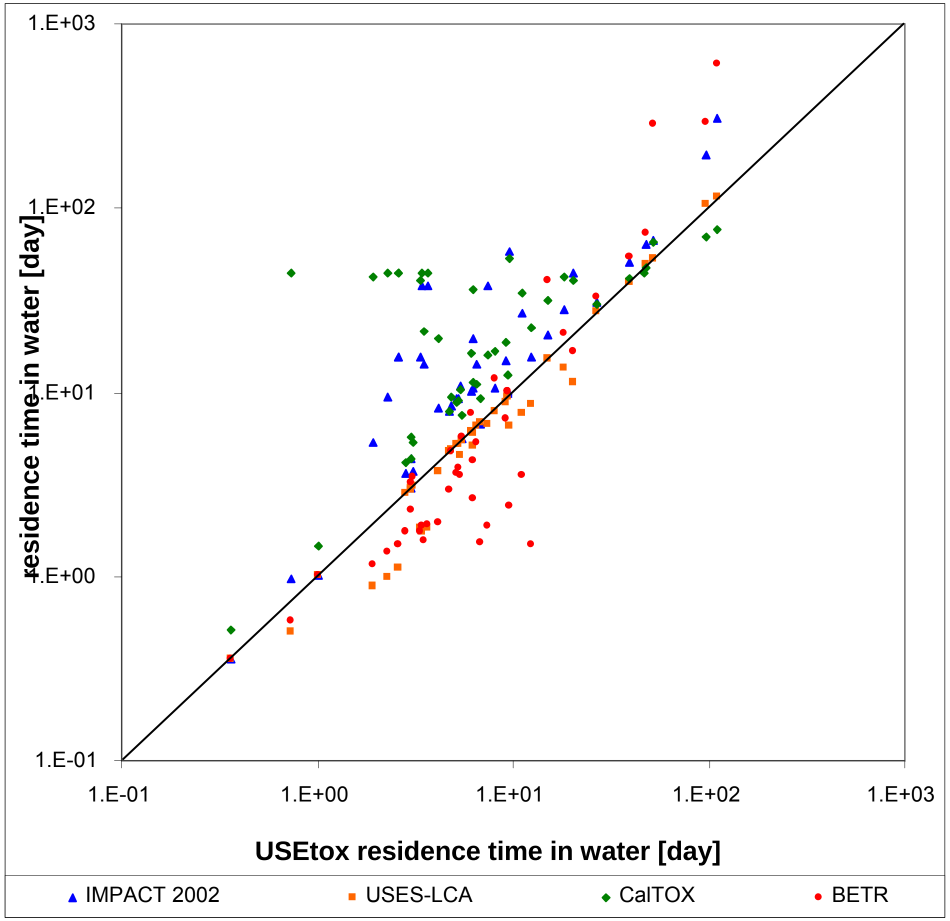


Ecotoxicity: CF=FF·EF

Human toxicity: CF=iF·EF

FFs Aquatic environment

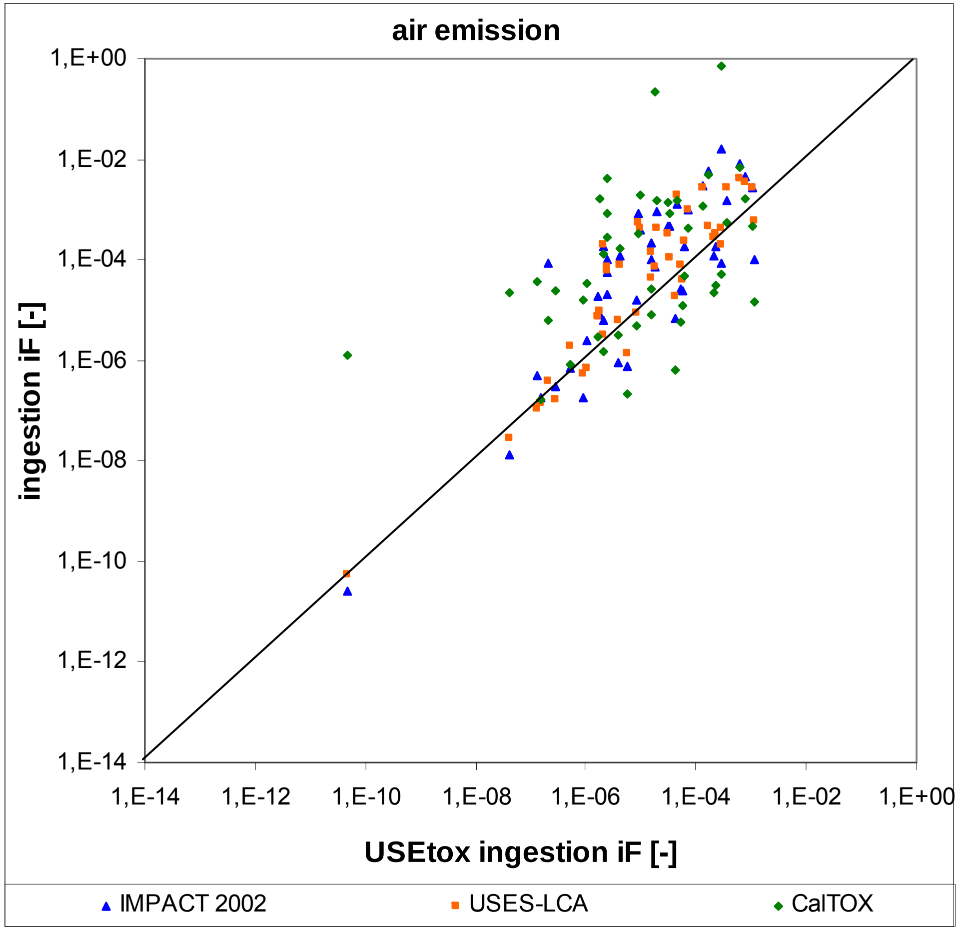




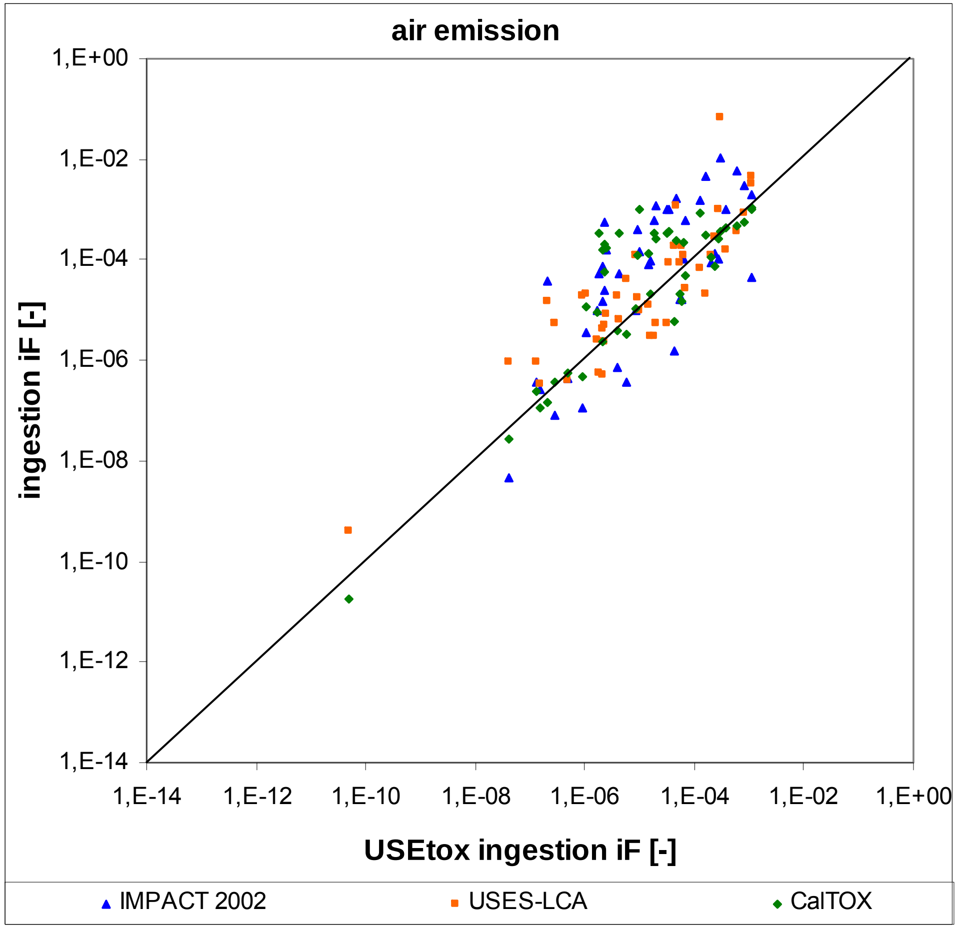
First workshop, Bilthoven

Final workshop, Montreal

IFs for ingestion

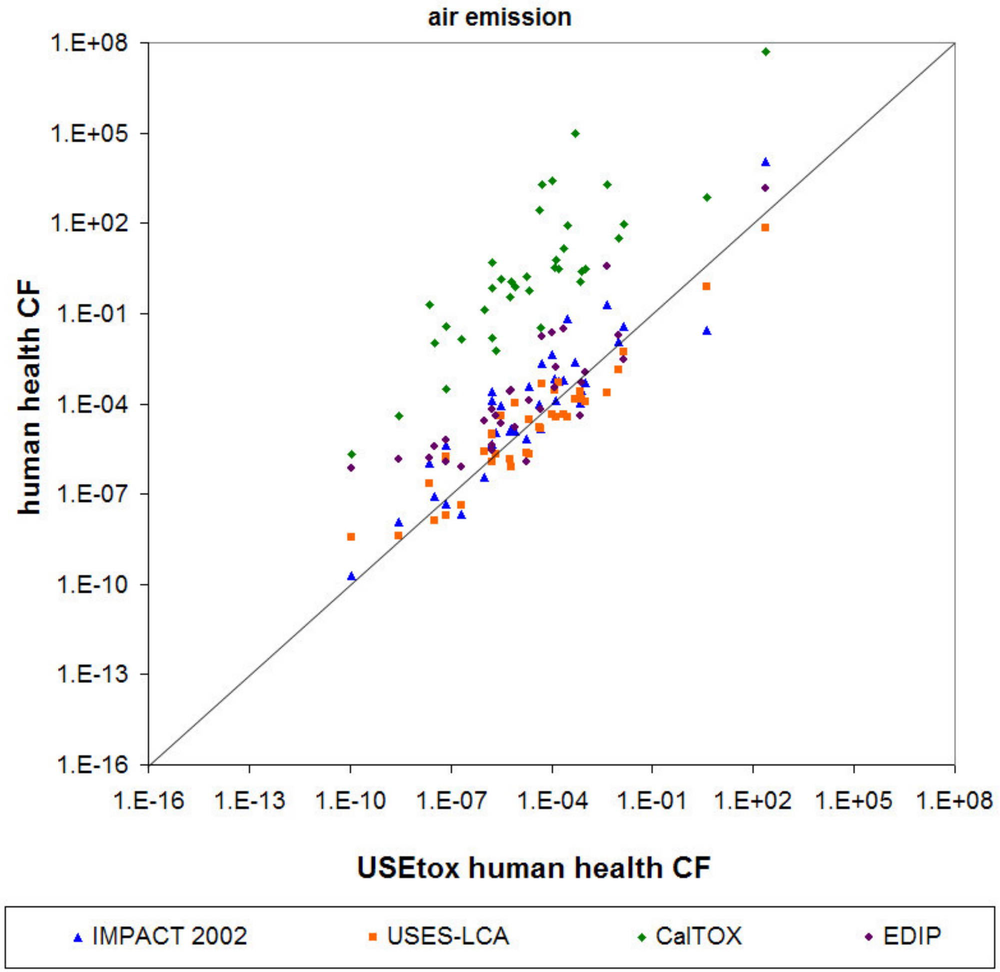


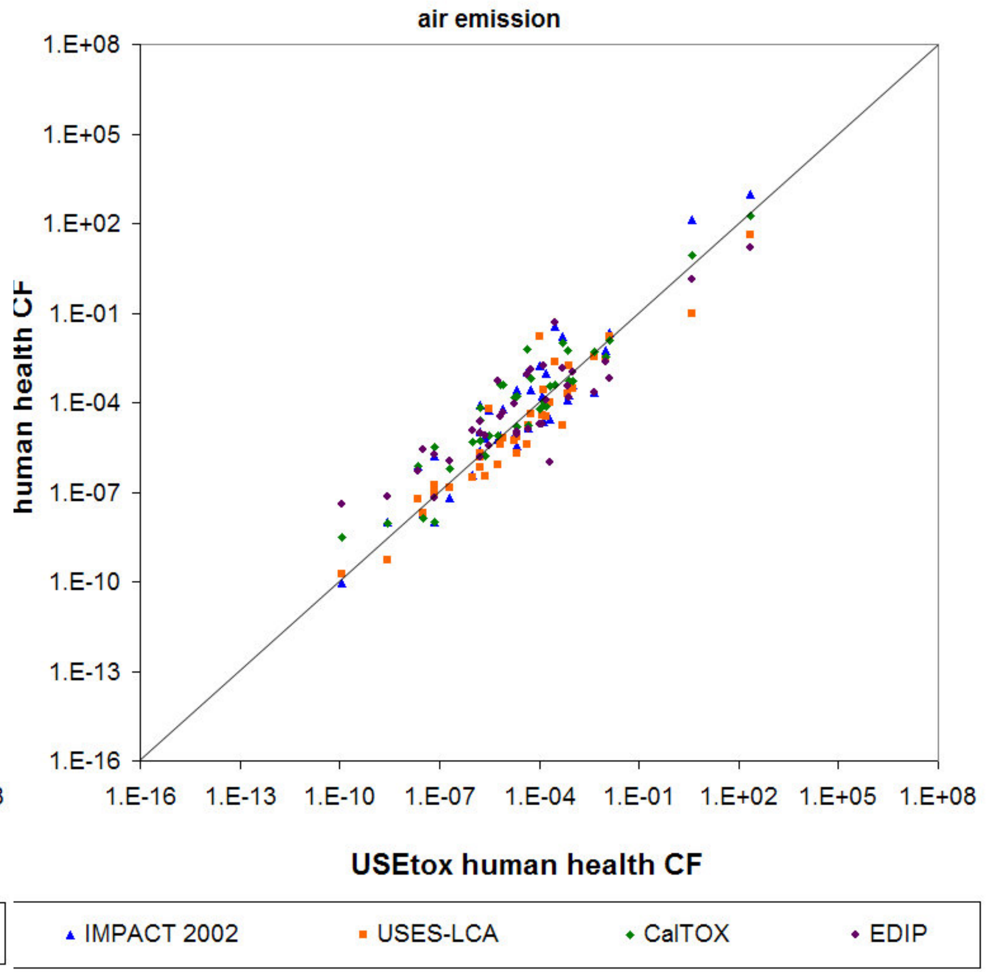
First workshop



Final workshop

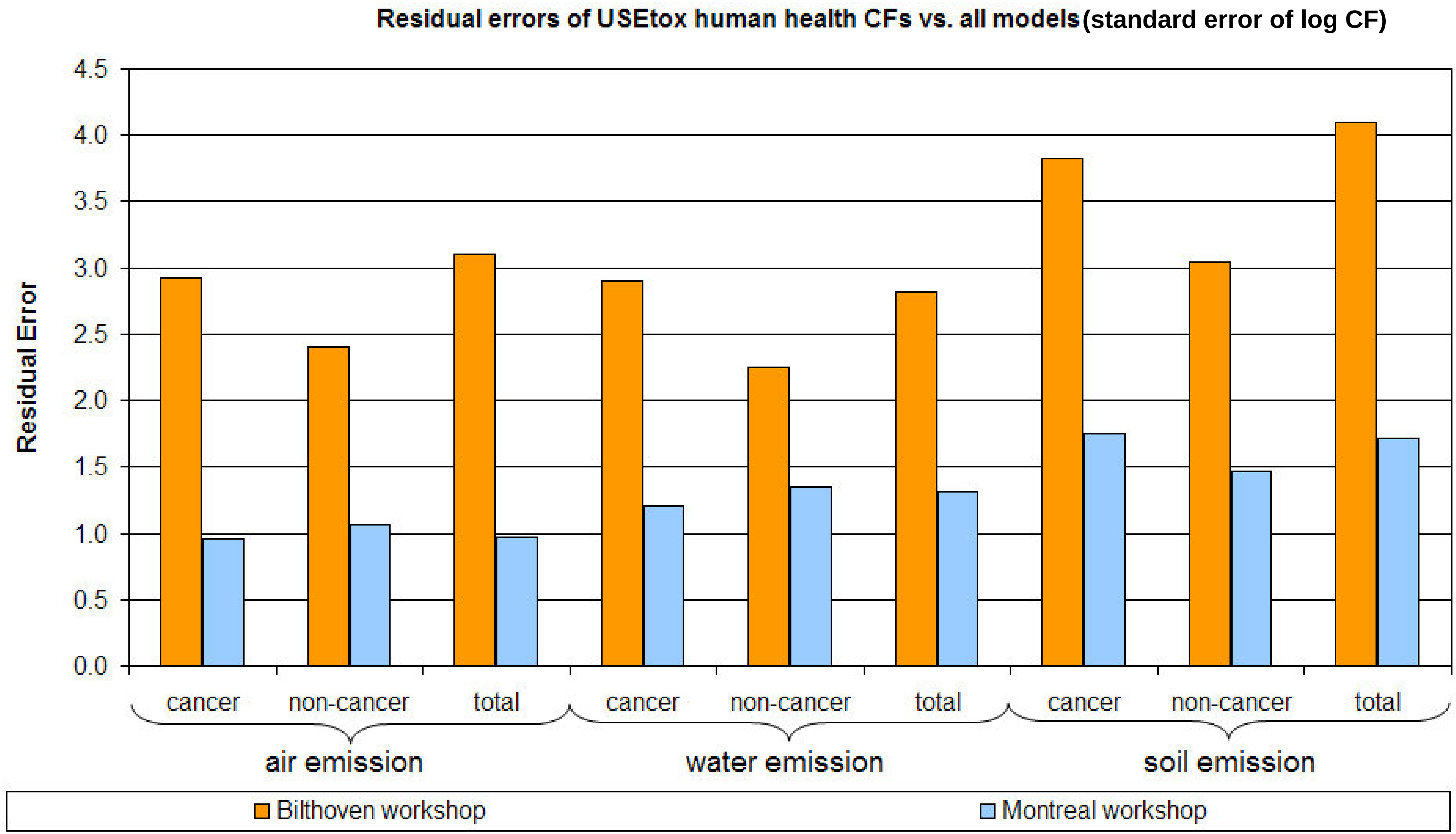
CFs Human health



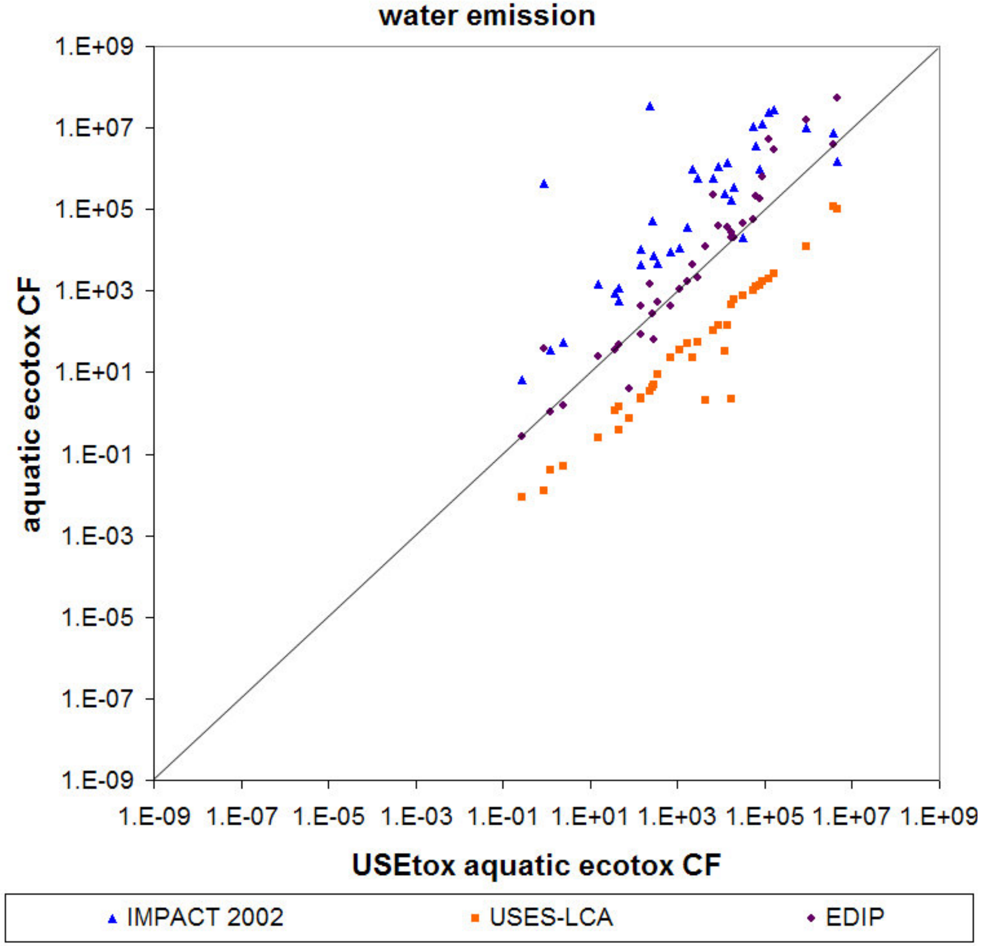


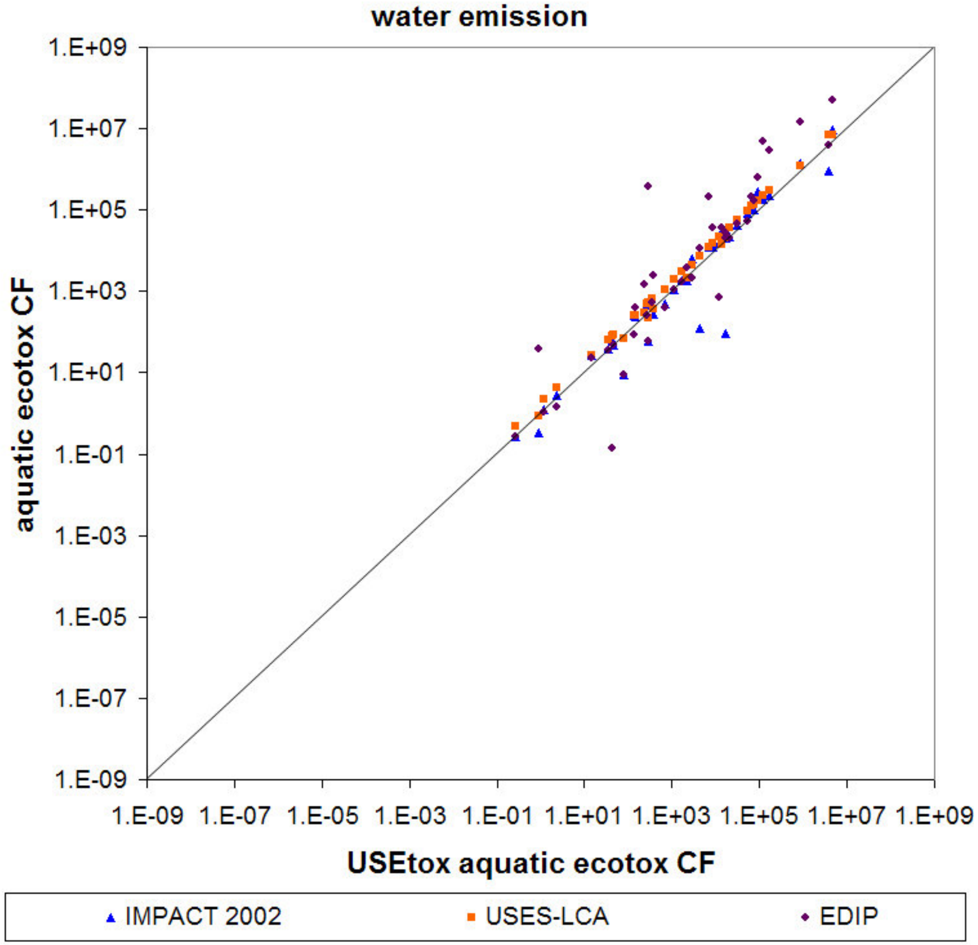
First workshop **Final workshop**

CFs Human toxicity



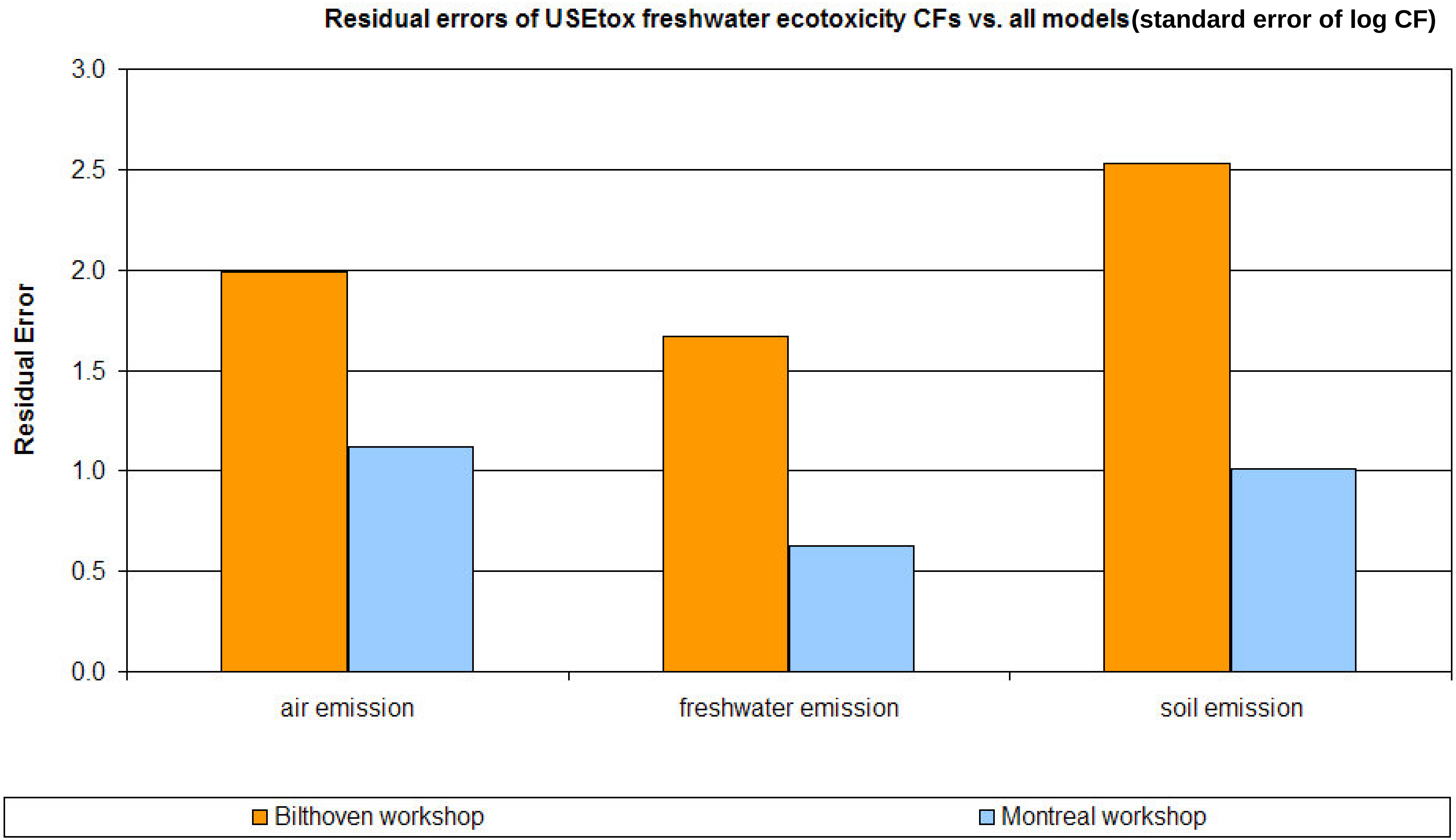
CFs Aquatic ecotoxicity





First workshop **Final workshop**

CFs Aquatic ecotoxicity



Conclusions

Harmonisation eliminates unintentional differences and considerably reduces variation between models.

Characterisation factors calculated with USEtox™ fall within range of the other models, even after their harmonisation.

Relative accuracy (model variability) of the new CFs is within a factor of

- 100-1000 for human health and
- 10-100 for freshwater ecotoxicity
- compared to 12 orders of magnitude variation between CFs.

CFs calculated with USEtox™:

- *recommended* factors for 1000 substances for human toxicity and 1300 substances for freshwater ecotoxic impacts
- *interim* factors for additionally 350 substances for human toxicity and 1250 substances (including metals) for freshwater ecotoxic impacts.

Outlook

USEtox™ and recommended CFs will be stable for at least 3-5 years though the other characterization models change.

Results are applicable to comparative chemical assessments also outside Life Cycle Impact Assessment, e.g.

- Ranking and prioritization of chemicals
- Chemical substitutions

Second phase of UNEP-SETAC Life Cycle Initiative (on-going):

- Metals targeted (freshwater, soil) to give realistic CFs
- USEtox™ will be made available in user-friendly version
- Substance data will be quality assured and parameter uncertainty estimated
- Case studies will be developed with chemical industry partners

Collaboration

The USEtox™ team invites partners from industry to collaborate on:

- Workshops to introduce and train the participants in use of the USEtox model
- Calculation of characterisation factors for other substances
- Development of cases demonstrating the relevance of:
  - looking at chemicals in life cycle perspective (e.g. chemical substitution)
  - including chemical impacts in life cycle assessments (*"carbon footprint does not say it all"*)

Please contact:

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More information

Hauschild, M.Z., Huijbregts, M., Jolliet, O., MacLeod, M., Margni, M., van de Meent, D., Rosenbaum, R.K. and McKone, T.: **Building a model based on scientific consensus for Life Cycle Impact Assessment of chemicals: the Search for Harmony and Parsimony.** *Environmental Science and Technology, 42(19), 7032-7037, 2008.*

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www.usetox.org (under construction)